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Plenary Session: Fluid Instabilities and Mixing in Extreme Conditions
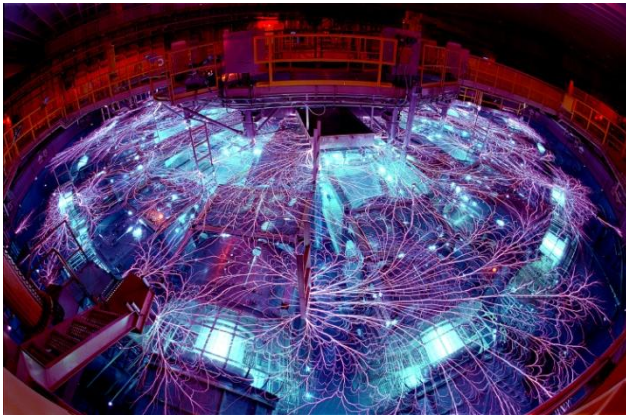
O. Schilling

January 7, 2011

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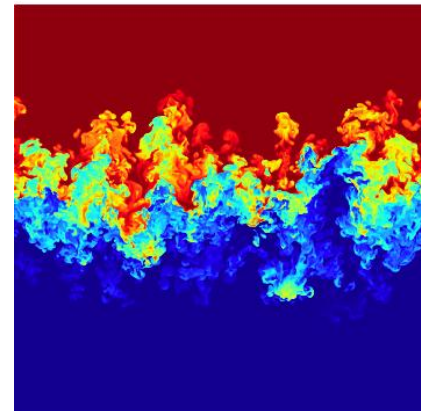
Presented at the
Research Needs for Material Mixing at Extremes Workshop
Santa Fe, New Mexico

Plenary Session:
Fluid Instabilities and Mixing in Extreme Conditions

10 January 2011
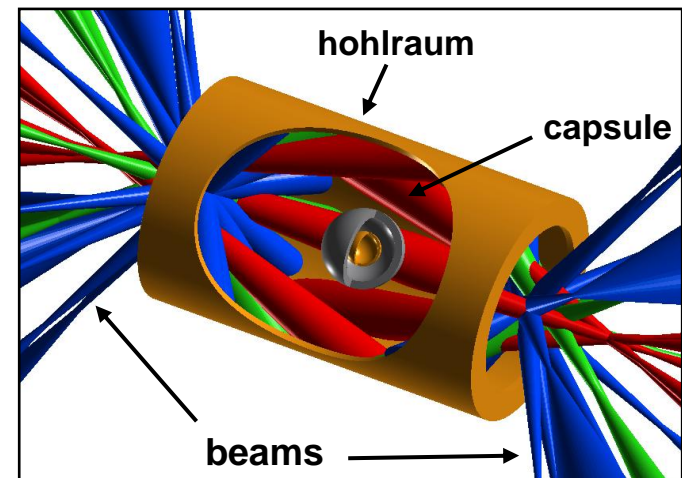
Oleg Schilling

LLNL-PRES-

Outline

- **Why are we interested in fluid instabilities and mixing?**

- **Brief description of Rayleigh–Taylor, Richtmyer–Meshkov, and Kelvin–Helmholtz instabilities**

- **Why has progress on understanding these instabilities and mixing processes been challenging?**

- **Overview of experiments: high- and low-energy-density**

- **Modeling objectives**

- **Overview of simulations (MILES/ILES, DNS, LES)**

- **Overview of Reynolds-averaged Navier–Stokes modeling**

- **Example of synergy between experiment, simulation, and modeling**

- **Data needed for model analysis, validation, and further development**
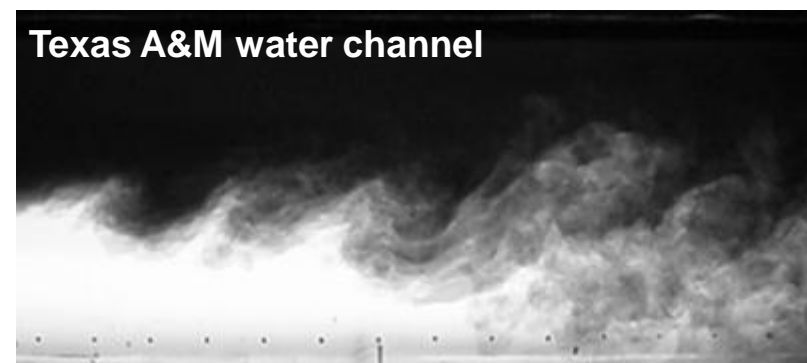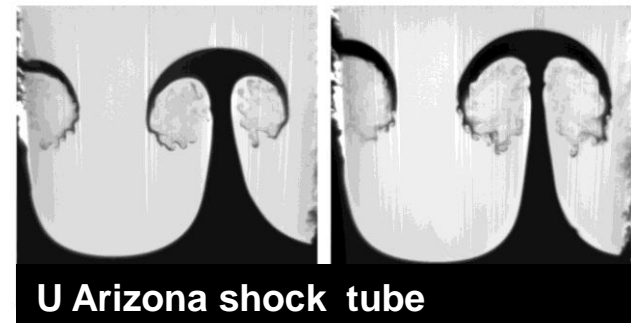
- **Vision**

Fluid instabilities and mixing are of fundamental as well as applied interest to high-energy-density phenomena such as inertial confinement fusion (ICF)

- **Fundamental fluid mechanics and low-energy-density applications**

  - **Ocean mixed layer and stratified turbulence**

  - **Atmospheric inversion**

  - **Atomization of droplets and sprays**

  - **Multiphase flows**

  - **Supersonic combustion**

  - **Turbulent reacting flows**

- **High-energy-density (extreme) applications**

  - **ICF (implosion, burning of DT fuel): see Jim Fincke's talk**

  - **Supernovae (explosion, thermonuclear flames): see Chris Fryer's talk**

  - **Interstellar turbulence (molecular clouds)**

Convective cloud formation

hohlraum

capsule

beams

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Two-fluid hydrodynamic instabilities are particularly relevant to ICF and to supernovae and result in fluid interpenetration and mixing

- **Rayleigh–Taylor (RT) instability** results from misaligned density and pressure gradients $\nabla p \bullet \nabla \rho < 0$

  - heavy fluid accelerated by a lighter fluid
  - baroclinic vorticity generation $\nabla p \times \nabla \rho / \rho^2$

- **Richtmyer–Meshkov (RM) instability** occurs when a shock traverses a perturbed interface

  - depositing vorticity on interface baroclinically
  - *reshock* deposits additional vorticity and compresses layer

- **Kelvin–Helmholtz (KH) instability** is driven by velocity shear

  - produces rollups with "mushroom" caps primarily on RT and RM spikes

Cold water → Flow direction
Warm water
Texas A&M water channel

U Arizona shock tube

Texas A&M water channel

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Hydrodynamic instability-induced turbulent mixing has a number of distinct features compared to more typical turbulent flows
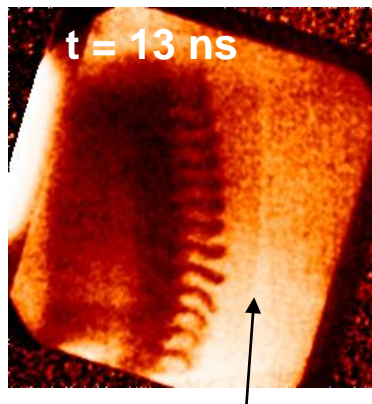
- **Anisotropy and inhomogeneity** from initial conditions, geometry, and preferred direction (time-varying accelerations or shocks)

- **Shocks and material discontinuities**

- **Baroclinic effects** due to vorticity production near interfaces due to misaligned *p* and ρ gradients

- **Two-fluid shear and mixing**, not single-fluid shear and mixing of a scalar

- **Varying density, locally strong compressibility** (e.g., during reshock) and **nonequilibrium**

- **Flow *transitional*, not fully-developed at early times**

- **Consideration of mixture properties** (equation of state, transport coefficients, etc.)

- **Reactions among species**

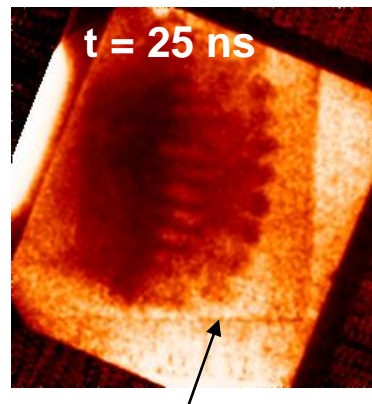- **Difficult to estimate order of magnitude and relative importance of terms *a priori***

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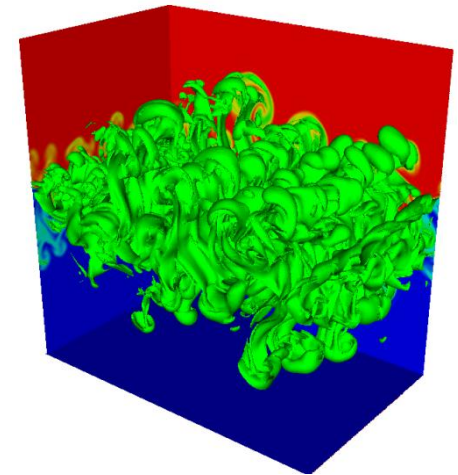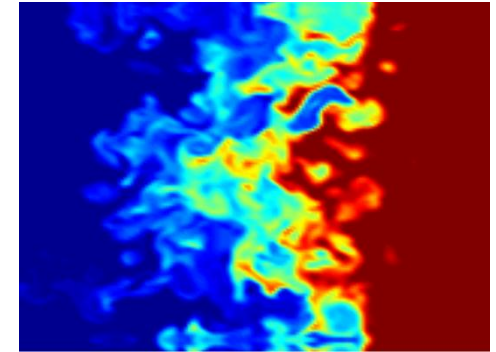
High-energy-density experiments on laser and Z-pinch facilities have been performed to better understand hydrodynamic instabilities

- **Experiments appear to be approaching a turbulent state, and exhibit differences with simulations**

- **Experiments limited by target size, which affects diagnostics, interface planarity, appearance of larger-scale structure etc.**

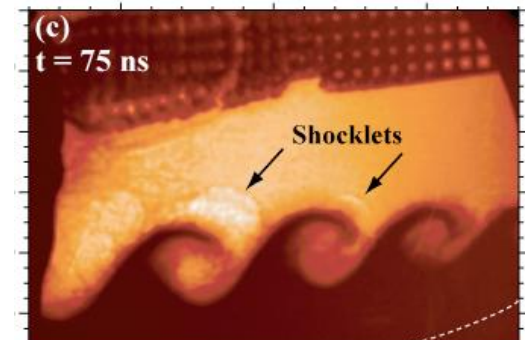- **Complex experiments involve many integrated effects and plasma conditions difficult to capture in simulations and by models**

OMEGA experiments on RT (below) and KH instability growth (right)
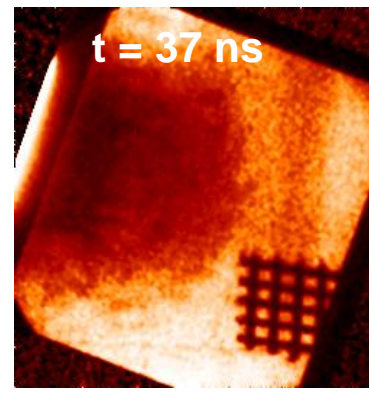

t = 13 ns

t = 25 ns

t = 37 ns

shock

shock-tube wall

(a) t = 25 ns — Blast wave, Unshocked CRF foam, 60 μm, Transmitted shock

(b) t = 45 ns

(c) t = 75 ns — Shocklets

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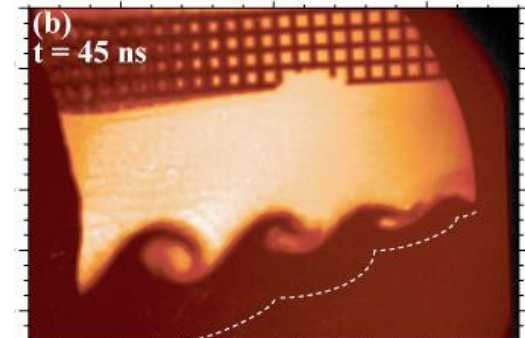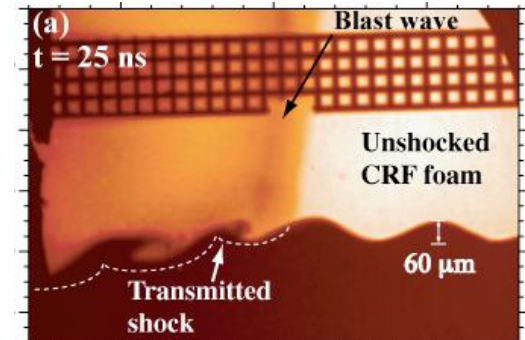
Low-energy-density experiments have begun to yield detailed data needed for simulation and model validation, but are in a limited regime

- They provide more detailed data and statistics using classical fluid diagnostic techniques —velocimetry, anemometry, fluorescence

- Rayleigh–Taylor experiments have progressed beyond imaging flow and mixing layer widths to
    - mean field profiles
    - energy spectra
    - mixing parameters
    - PDFs

- Richtmyer–Meshkov experiments have progressed to
    - later times
    - higher Mach numbers
    - mixing statistics and profiles

- **However, this data is incomplete and is challenging to acquire over a broad range of physical parameters**

Images of transition from LANL gas curtain experiments

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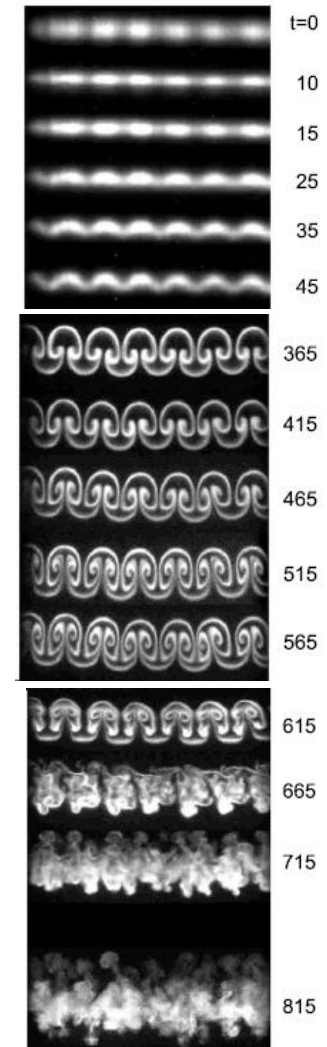
An important objective is the development of reduced descriptions of turbulent mixing that balance accuracy with cost effective simulations

- **Reduced models must account for discussed flow complexities and:**
    - **broad spectrum of initial conditions (modes) and range of scales**
    - **regimes spanning many orders of magnitude:**
      Re ~ 0–10^8, A ~ 10^{-4}–1, Sc ~ 10^{-4}–10^3
- **DNS: resolve all scales**
    - **No averaging**
    - **Full 3D data available for all fields that can be averaged further**
- **MILES/ILES/LES: resolve "largest" scales**
    - **"Filter" full equations and model unclosed correlations (smaller, unresolved scales) using resolved-scale data**
    - **Only resolved fields available**
- **RANS: model all scales**
    - **Ensemble average equations and model unclosed correlations using mean field data**
    - **Turbulent transport equations needed for closures**

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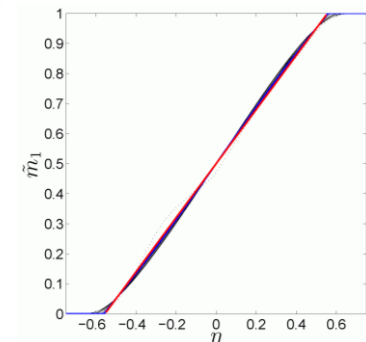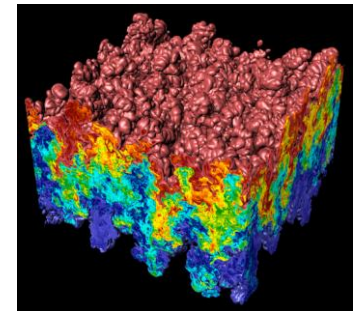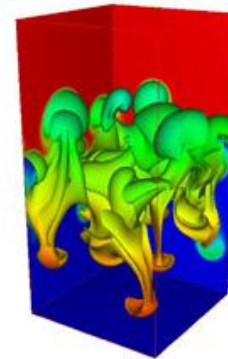
The approaches used to simulate hydrodynamic instabilities and mixing have important limitations

- **Monotone integrated/implicit LES** (MILES/ILES) relies on numerical dissipation (e.g., simulations of nondissipative equations) which is not well understood
  - **Advantages**: modest computational requirements, large-scale structures and lowest-order integral properties generally well captured, no consideration of transport coefficients, no explicit averaging
  - **Disadvantages**: small-scale structures not estimated correctly, results grid dependent and do not converge, "mixing" is numerical, Sc effects not captured
- **LES** relies on modeled dissipation
  - **Advantages**: less costly than DNS, less modeling than required by RANS, results can be interpreted as an ensemble average
  - **Disadvantages**: only meaningful in 3D, requires high quality algorithms, depends on grid resolution and on details of subgrid models, formulation of large-eddy equations nontrivial for complex flows with multiphysics
- **DNS** relies on physical dissipation
  - **Advantage**: all structures and statistics estimated well with appropriate resolution and a sufficiently large ensemble
  - **Disadvantages**: <u>very high</u> computational and data storage/processing requirements, only meaningful in 3D, requires high quality algorithms, problematic when discontinuities present

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RANS modeling of hydrodynamic instabilities and mixing also has important limitations

- **Reynolds-averaged Navier–Stokes** (RANS) models rely on modeled turbulent transport equations to provide closures

  - **Advantages**: modest computational and resolution requirements, can be used in 3D/2D/1D, results are ensemble averaged, can be implemented in nearly any underlying hydrodynamics algorithm

  - **Disadvantages**: closures needed for many terms, closures are based on gradient-diffusion and similarity, proliferation of transport equations and model coefficients, difficult to model physical effects using common coefficient sets, largely postdictive requiring different coefficients for different flows, dependence on initial conditions, models do not naturally "turn off" as resolution increases towards LES/DNS resolutions

Many quantities in the Reynolds-averaged equations require closure, which can be achieved at various levels of complexity

- **Reynolds stresses** $\tau_{ij} = \overline{\rho}\,\widetilde{u_i'' u_j''}$ **, turbulent fluxes such as**

  $\overline{\rho}\,\widetilde{u''^2 u_j''}$, $\overline{p' u_j''}$, $\overline{\rho}\,\widetilde{m_1'' u_j''}$ **, averaged Favre fluctuating velocity (mass flux)**

  $\overline{u_j''} = -\overline{\rho' u_j'}/\overline{\rho}$ **, correlations (usually neglected)** $\overline{\sigma_{ij}'' u_i''}$, $\overline{h_r'' J_{r,j}''}$

- **A hierarchy of possible RANS closures is possible**

  - **2-equation models based on transport equations for K and ε (or L)**

  - **2nd-order closures based on transport equations for second moments such as τ_{ij} (BHR-3)**

  - **Intermediate models where production terms are transported (BHR-2)**

  - **Algebraic stress models based on simplifications of second moment equations**

- **Other modeled transport equations can be added to describe scalar mixing**

  - **Probability density function (PDF) methods can have a very useful role**

  - **Very well developed in combustion community, but only beginning to emerge for flows discussed here**

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The mean flow and turbulence equations are typically closed using empirical gradient-diffusion and similarity approximations

- **Gradient-diffusion approximation**

  - $\overline{\phi'_\alpha \phi'_\beta} = -\dfrac{\nu_t}{\sigma_{(\alpha\beta)}} \dfrac{\partial \overline{\phi}_\alpha}{\partial x_\beta}$ [$\sigma_{(\alpha\beta)}$ is a **model coefficient**] with turbulent viscosity

  $$\nu_t = C_\mu \frac{K^2}{\epsilon} \text{ or } \nu_t = C_\mu \sqrt{K}\, L$$

- **Similarity assumption** is used to model ε or L equation, in which each term is proportional to term in K equation but evolving on a timescale K/ε with an associated coefficient

- Mass flux is an important quantity appearing in K and ε or L equations

  - **Algebraic model** $\overline{u''_j} = \dfrac{\nu_t}{\sigma_\rho\, \overline{\rho}} \dfrac{\partial \overline{\rho}}{\partial x_j}$

  - **Two-fluid model** $\overline{u''_j} = \dfrac{f_1 f_2 (\rho_1 - \rho_2)(\tilde{u}_{j,1} - \tilde{u}_{j,2})}{\overline{\rho}}$

  - **Transport equation**
  $$\overline{\rho}\left(\frac{\partial}{\partial t} + \tilde{u}_j \frac{\partial}{\partial x_j}\right)\overline{u''_i} = -b\frac{\partial \overline{p}}{\partial x_i} + \frac{\tau_{ij}}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial x_j} - \overline{\rho}\,\overline{u''_j}\frac{\partial}{\partial x_j}\left(\tilde{u}_i + \overline{u''_i}\right)$$
  $$-\overline{\rho}\frac{\partial}{\partial x_j}\left(\overline{u''_i u''_j}\right) - C_{a2}\frac{\overline{\rho}\,\overline{u''_i}\sqrt{K}}{L} + \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_a}\frac{\partial \overline{u''_i}}{\partial x^j}\right)$$

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Ensemble-averaged descriptions cannot represent/describe many phenomena in turbulent flows

- **Intermittency and strongly non-Gaussian effects**
  - **may not have significant effects on large-scale transport**
  - **but may affect mixing properties**
- **Small-scale flow structure** (e.g., a complex interface in a mixing layer), as these diffusive models smooth out such structure
- <u>Standard</u> **2-equation models based on a *linear stress–strain relation* cannot model**
  - **nonequilibrium effects** (production <u>not</u> balanced by dissipation)
  - **rotational strains**
  - **Reynolds stress anisotropies**
  - **Reynolds stress component relaxation and growth**
- *Nonlinear* **(i.e., non-Boussinesq) and second-order closure models can potentially address many of these shortcomings**
  - **However, these are not particularly well developed for hydrodynamic instability-induced turbulence**

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Second-order closures explicitly model transport equations for second moments, rather than using gradient-diffusion modeling

- **Reynolds stress transport equation solved directly for τ_{ij} avoiding Boussinesq model**

  - **Production terms treated exactly**

  - However, τ_{ij} transport equation must be modeled

- **Exact transport equation**

$$\frac{\partial \tau_{ij}}{\partial t} + \frac{\partial}{\partial x_k}(\tau_{ij}\,\widetilde{u}_k) = -\overline{u_i''}\frac{\partial \overline{p}}{\partial x_j} - \overline{u_j''}\frac{\partial \overline{p}}{\partial x_i} - \tau_{ik}\frac{\partial \widetilde{u}_j}{\partial x_k} - \tau_{jk}\frac{\partial \widetilde{u}_i}{\partial x_k}$$

$$+ \overline{p'\left(\frac{\partial u_j''}{\partial x_i} + \frac{\partial u_i''}{\partial x_j}\right)} - \overline{\rho}\,\widetilde{\epsilon_{ij}''}$$

$$- \frac{\partial}{\partial x_k}\left(\overline{\rho}\,\widetilde{u_i''\,u_j''\,u_k''} + \overline{p'\,u_i''\,\delta_{jk} + p'\,u_j''\,\delta_{ik}} - \overline{\sigma_{ik}\,u_j''} - \overline{\sigma_{jk}\,u_i''}\right)$$

  contains averaged Favre fluctuating velocity, pressure–strain correlation, dissipation rate tensor, and triple correlation (turbulent diffusion), which must be modeled

- **These terms require even more detailed experimental and simulation data**

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An example of synergy between experiment, simulation and modeling is the evolution of RT mixing in a water channel predicted by DNS and RANS

- **Initial velocity/interfacial perturbations were taken from experimental data**

- **Optimized RANS model obtained by correlating DNS and model profiles *a priori* was tested *a posteriori***

- **Despite "simplicity" of this flow, computational and modeling limitations still result in discrepancies with measurements of molecular mixing θ**

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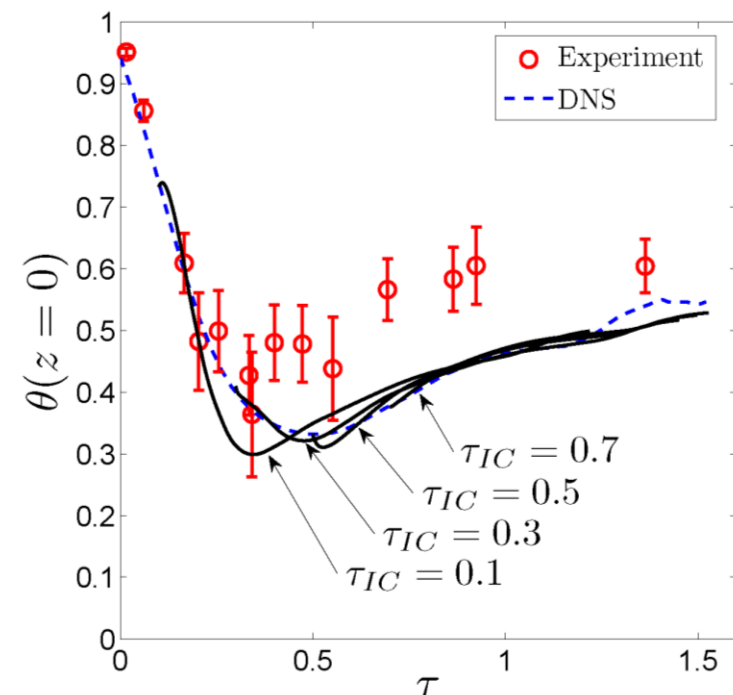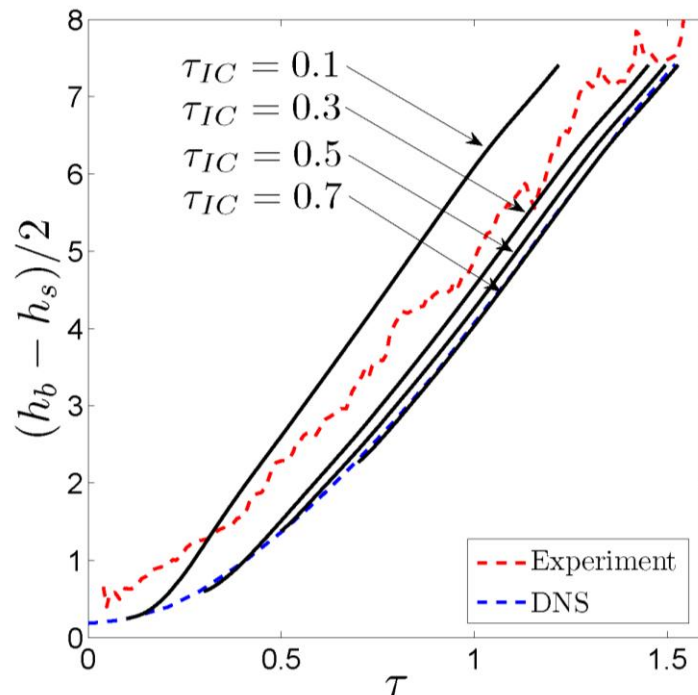
Quantities needed for model development and validation, and the experiments and simulations that can address them, are being identified

- **Progress in model development for hydrodynamic instability-generated turbulent mixing requires a broad array of detailed data**
  - **Smaller-scale data, turbulence statistics, and model terms in equations needed in addition to large-scale data**
  - **Desirable to have (x,t) data for correlations of turbulent quantities and spectra, in addition to profiles**
  - **Data on compressibility effects at larger *Ma*, and on transitional, anisotropic effects**
  - **Measurements addressing production terms are most important**
- **Push limits on diagnostics and spatiotemporal resolution: is there a role for holographic and tomographic techniques?**
- **Better coordinate simulations, experiments, and models (measurement of initial conditions etc.)**
- **Generate datasets for validation using accurate methods suitable for flows with material discontinuities and shocks**
- **Perform *a priori* and *a posteriori* tests of integrated and detailed model predictions**

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Increasing computational and experimental capabilities applied to fluid instabilities and mixing will continue to better "inform" models

- **Codes used for ICF design and interpretation of experimental results drive modeling requirements**
  - **Models are tightly coupled to hydrodynamics, imposing constraints on types and details of suitable models**
  - **RANS models are likely to be short- and intermediate-term approaches to turbulence modeling**
- **Experiments and simulations have limitations but are indispensible**
  - **Establish where models give good and poor predictions**
  - **Better understand successes and shortcomings of models**
- **For enhanced predictive capability, it is desirable to numerically resolve more and model less physics**
- **There is an expanding role for LES and hybridization with RANS models to address hydrodynamic instability generated turbulence**
- **High quality, detailed experimental data is needed for *both* RANS and LES**
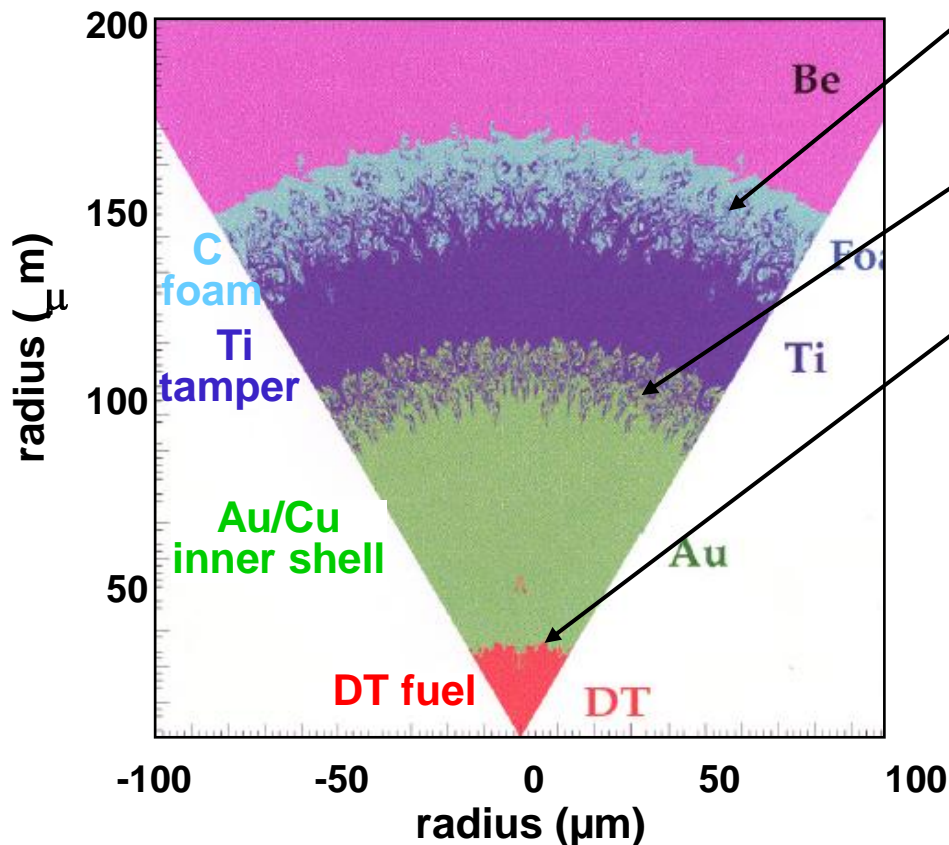
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Backup slides

Double-shell capsules are promising for ICF, but are highly susceptible to Rayleigh–Taylor and Richtmyer–Meshkov instabilities

**2D HYDRA simulation of NIF-scale ignition double shell capsule (modes 12–816)**

- **Initial short-scale (surface roughness) and long-scale (drive asymmetries) perturbations**
- **Several unstable interfaces with multiple shock interactions and reshock; compressible: *Ma* ~ 10**
- **Inner-shell/fuel interface RT unstable upon deceleration**
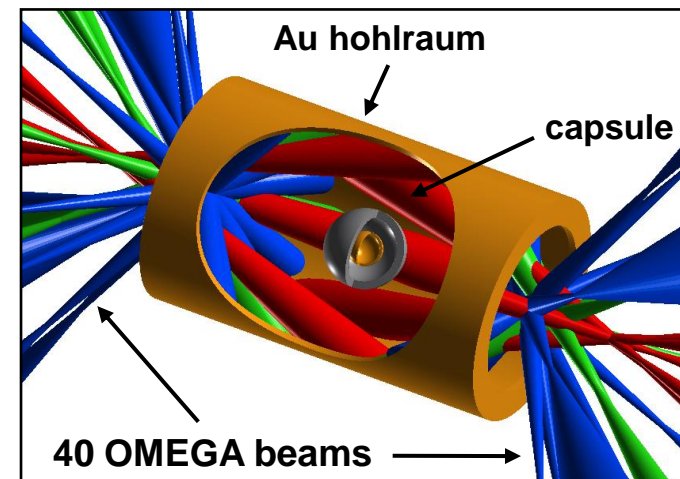
Compressible turbulent mixing is also prevalent in astrophysics, such as in supernovae implosions and explosions

- **Thermonuclear fuel is eventually exhausted in a star**
  - **Collapse ensues as internal pressure generated by fusion no longer balances inward gravity**
  - **A sequence of fusion reactions is initiated, ultimately producing Fe and terminating reaction sequence**
- **Subsequent collapse generates a <u>strong shock</u> which**
  - **rebounds from imploding core**
  - **propagates outward resulting in mass ejection: type II supernova remnant**
- **Stratified material interfaces (O-He and He-H) are classically RT, RM, and KH unstable**

Simulation of SN1987A at t = 3.6 hr

shock front
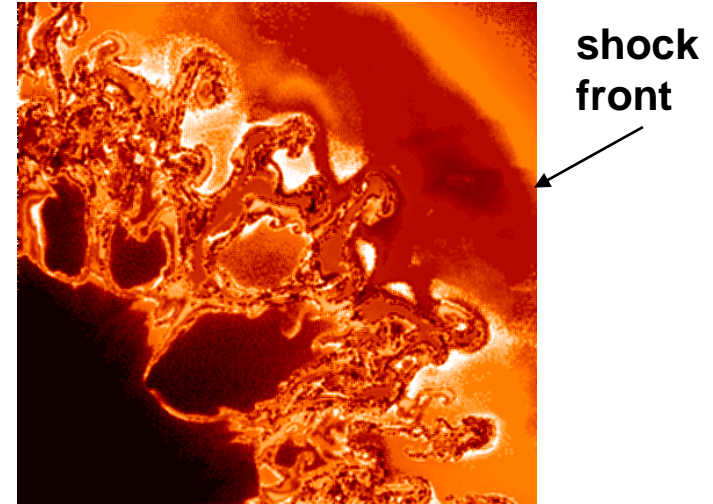
Müller, E., Fryxell, B. & Arnett, D. 1991 Instability and clumping in SN1987A. *Astron. Astrophys.* 251, 505

2D simulations:
- **predict that heavy fluid spikes propagate ahead of interface due to RM and RT instabilities**
- **underpredict ^{56}Ni velocities by ~ 2**

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RANS models are based on statistically-averaging the single-velocity multicomponent flow equations and require closure

- **Ensemble averaging equations gives (consider binary ideal gases with a single scalar mass fraction and nonreacting flow)**

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_j}(\overline{\rho}\,\widetilde{u}_j) = 0$$

$$\frac{\partial}{\partial t}(\overline{\rho}\,\widetilde{u}_i) + \frac{\partial}{\partial x_j}(\overline{\rho}\,\widetilde{u}_i\,\widetilde{u}_j + \overline{p}\,\delta_{ij}) = \overline{\rho}\,g_i + \frac{\partial \overline{\sigma}_{ij}}{\partial x_j} - \underbrace{\frac{\partial \tau_{ij}}{\partial x_j}}$$

$$\frac{\partial}{\partial t}(\overline{\rho}\,\widetilde{e}) + \frac{\partial}{\partial x_j}[(\overline{\rho}\,\widetilde{e} + \overline{p})\,\widetilde{u}_j] = \overline{\rho}\,g_i\,\widetilde{u}_i + \frac{\partial}{\partial x_j}(\overline{\sigma}_{ij}\,\widetilde{u}_i) + \frac{\partial}{\partial x_j}\left(\overline{K}\,\frac{\partial \widetilde{T}}{\partial x_j} - \sum_{r=1}^{2}\widetilde{h}_r\,\widetilde{J}_{r,j}\right) - \frac{\partial}{\partial x_j}\left(\sum_{r=1}^{2}\underbrace{\overline{h_r''\,J_{r,j}''}}\right)$$

$$- \frac{\partial}{\partial x_j}\left(\underbrace{\frac{\overline{\rho\,u''^2\,u_j''}}{2}} + \underbrace{\tau_{ij}}\,\widetilde{u}_i + \underbrace{\frac{\overline{p}\,\overline{u_j''}}{\gamma - 1}} + \underbrace{\frac{\overline{p'\,u_j''}}{\gamma - 1}}\right) - \frac{\partial}{\partial x_j}\left(\underbrace{\overline{p'\,u_j'' - \sigma_{ij}''\,u_i''}}\right)$$

$$\frac{\partial}{\partial t}(\overline{\rho}\,\widetilde{m}_1) + \frac{\partial}{\partial x_j}(\overline{\rho}\,\widetilde{m}_1\,\widetilde{u}_j) = \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\overline{D}\,\frac{\partial \widetilde{m}_1}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left(\underbrace{\overline{\rho\,m_1''\,u_j''}}\right)$$

- **Quantities with underbraces are unclosed and require modeling**

A DNS[1] modeling a water channel Rayleigh–Taylor mixing experiment at Texas A&M[2] was performed using the MIRANDA code

$L_x \times L_y \times L_z$	28.8 cm $\times$ 18 cm $\times$ 24 cm
$N_x \times N_y \times N_z$	1152 $\times$ 720 $\times$ 1280
A	7.5×10^{-4}
ρ_1	0.9986 g/cm^3
ρ_2	0.9970 g/cm^3
g	981 cm/s^2
Sc (Pr)	7.0

g
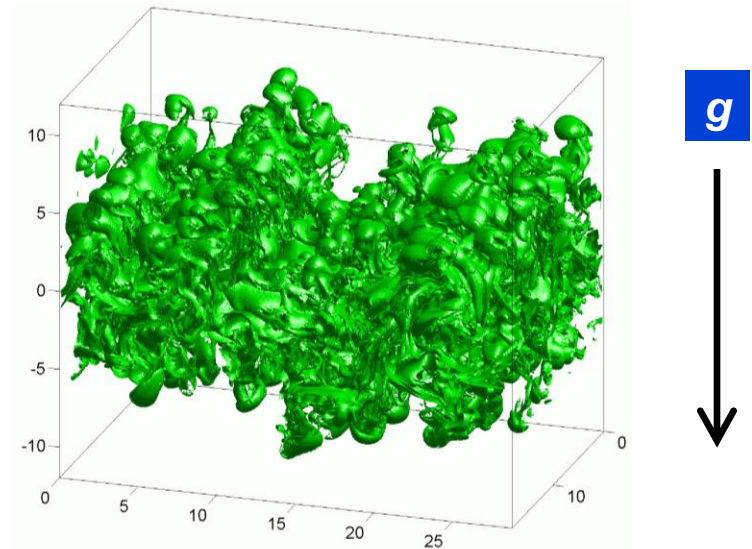
- **Initial velocity/interfacial perturbations taken from experimental data**

- **At latest time, integral-scale Reynolds number reaches ~ 4500**

[1] N. J. Mueschke & O. Schilling, "Investigation of Rayleigh–Taylor turbulence and mixing using direct numerical simulation with experimentally measured initial conditions. I. Comparison to experiment, II. Dynamics of transitional flow and mixing statistics ," *Phys. Fluids* 21, 014106, 014107 (2009a,b)

[2] N. J. Mueschke, M. J. Andrews & O. Schilling, "Experimental characterization of initial conditions and spatio-temporal evolution of a small Atwood number Rayleigh–Taylor mixing layer," *J. Fluid Mech.* 567, 27 (2006)

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The initial velocity and interfacial perturbations were parameterized from experimental data

- **Interface perturbed in *x*- and *y*-directions** $\zeta(x,y) = \sum_{k_x} \widehat{\zeta}_x \, e^{i\,k_x\,x} + \sum_{k_y} \widehat{\zeta}_y \, e^{i\,k_y\,y}$

- **Velocity field constructed from perturbed potential field**

$$\phi_r(x,z) = \sum_{k_x} \frac{\widehat{w}(k_x)}{k_x} e^{i\,k_x\,x}\, e^{-k_x\,|z|} \qquad u_i = \frac{\partial \phi_r}{\partial x_i} - \frac{D}{\rho}\frac{\partial \rho}{\partial x_i}$$
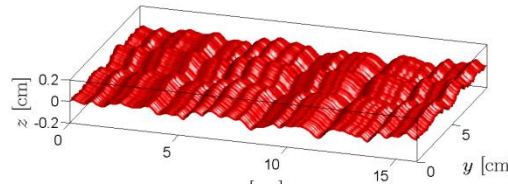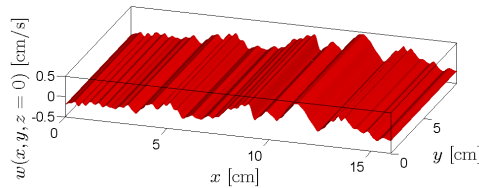

**Initial density interface and vertical velocity at centerplane**

x-direction velocity perturbation

x-direction interfacial perturbation

y-direction interfacial perturbation
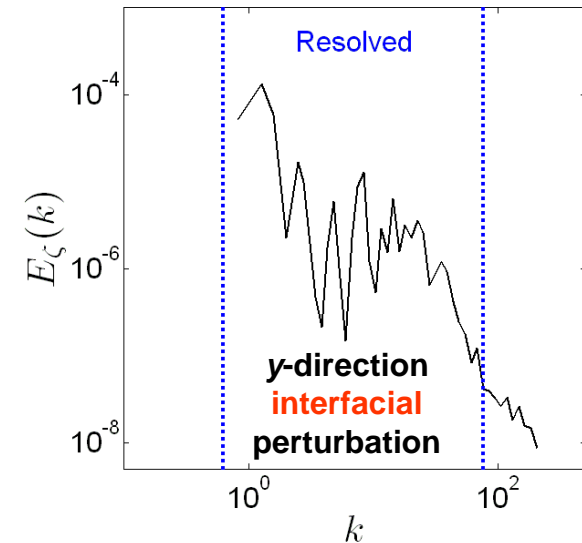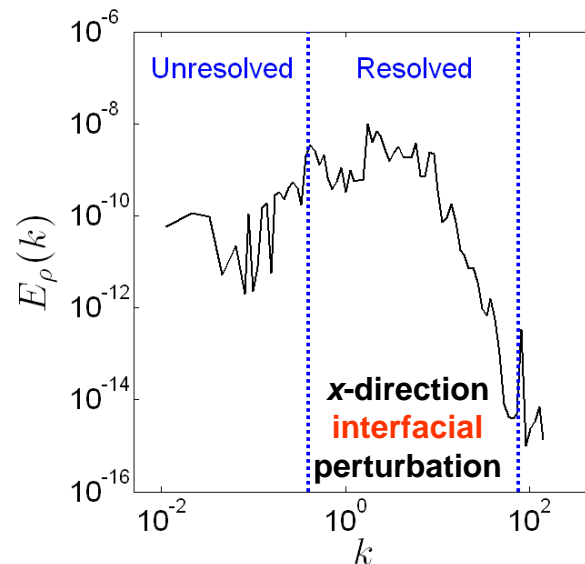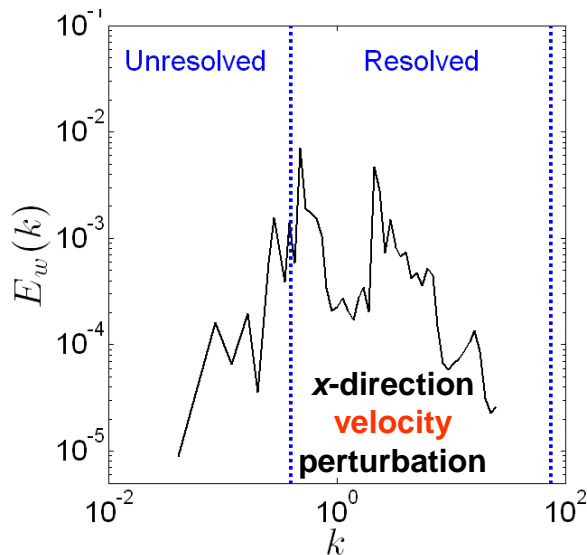
The growth of the mixing layer and the evolution of the molecular mixing parameter predicted by a RANS model compare favorably with DNS

- **Optimized RANS model obtained by correlating DNS and model profiles was tested *a posteriori* using a 1D numerical implementation**

- **Model initialized using DNS data at times τ_{IC} = 0.1, 0.3, 0.5, 0.7 to test early-time model dynamics**

- **For τ > 0.8, all model instantiations give very similar layer growth and θ**
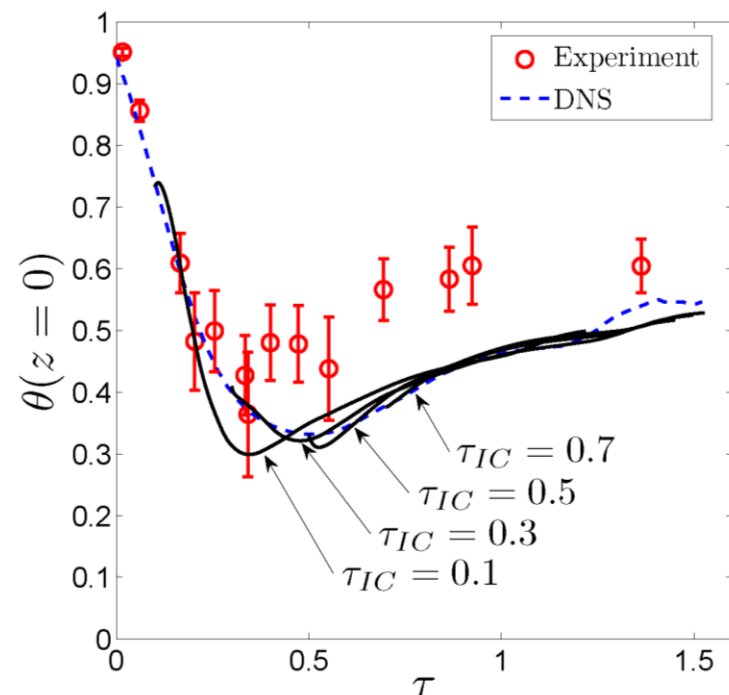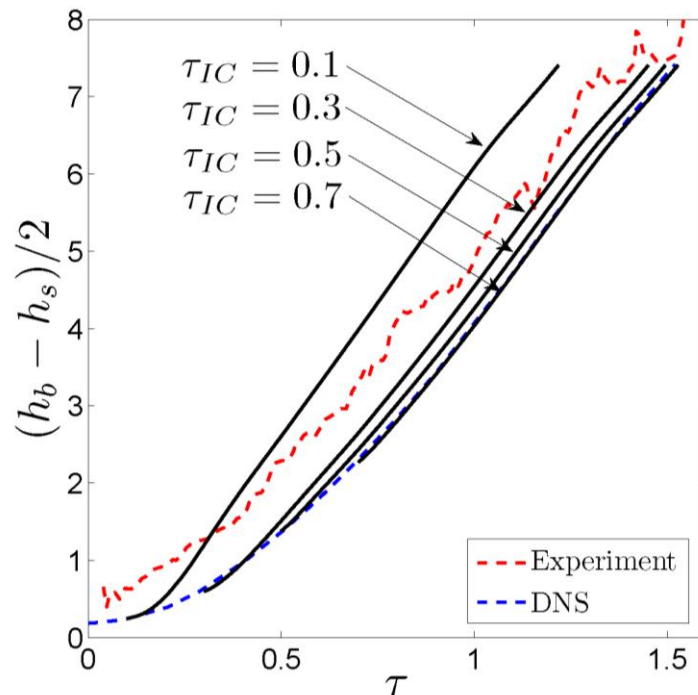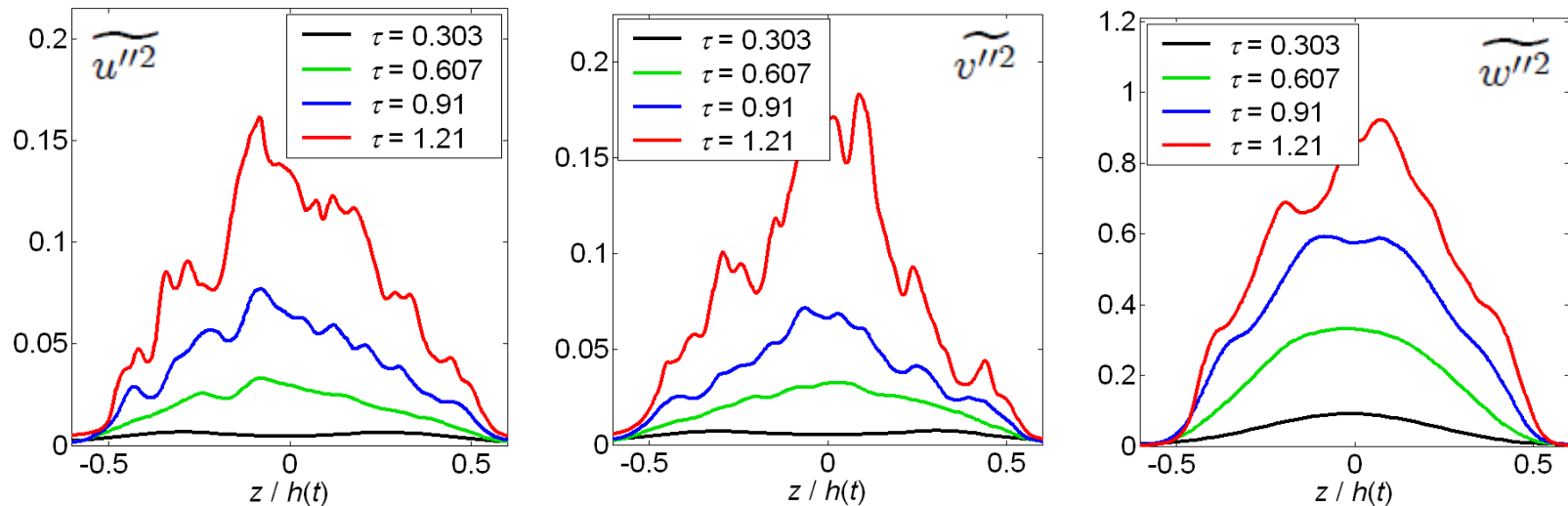
This DNS has yielded insight into the role of complex initial conditions

Evolution of mass fraction one-half isosurface colored by buoyancy production

$\tau = 0.25$ $\tau = 0.50$ $\tau = 0.75$ $\tau = 1.00$
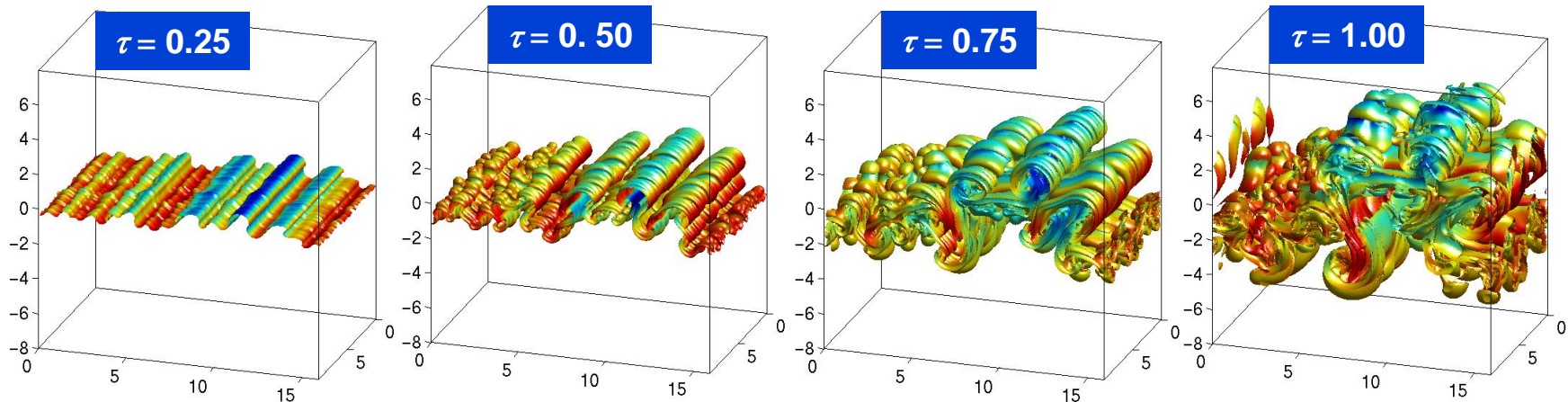
Evolution of velocity variances

Simulations of Richtmyer–Meshkov instability modeling the Vetter–Sturtevant experiment have yielded insight into turbulence amplification by reshock

reshock

t = 3 ms t = 3.25 ms t = 3.5 ms t = 7 ms